

Efficient non-linear proper orthogonal decomposition/Galerkin reduced order models with stable penalty enforcement of boundary conditions

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SUMMARY

An efficient, stability-preserving model reduction technique for non-linear initial boundary value problems whose solutions exhibit inherently non-linear dynamics such as metastability and periodic regimes (limit cycles) is developed. The approach is based on the ‘continuous’ Galerkin projection approach in which the continuous governing equations are projected onto the reduced basis modes in a continuous inner product. The reduced order model (ROM) basis is constructed via a proper orthogonal decomposition (POD). In general, POD basis modes will not satisfy the boundary conditions of the problem. A weak implementation of the boundary conditions in the ROM based on the penalty method is developed. Asymptotic stability of the ROM with penalty-enforced boundary conditions is examined using the energy method, following linearization and localization of the governing equations in the vicinity of a stable steady solution. This analysis, enabled by the fact that a continuous representation of the reduced basis is employed, leads to a model reduction method with an *a priori* stability guarantee. The approach is applied to two non-linear problems: the Allen–Cahn (or ‘bistable’) equation and a convection-diffusion-reaction system representing a tubular reactor. For each of these problems, bounds on the penalty parameters that ensure asymptotic stability of the ROM solutions are derived. The non-linear terms in the equations are handled efficiently using the ‘best points’ interpolation method proposed recently by Peraire, Nguyen *et al.* Numerical experiments reveal that the POD/Galerkin ROMs with stability-preserving penalty boundary treatment for the two problems considered, both without as well as with interpolation, remain stable in a way that is consistent with the solutions to the governing continuous equations and capture the correct non-linear dynamics exhibited by the exact solutions to these problems. Published 2012. This article is a US Government work and is in the public domain in the USA.

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1. INTRODUCTION

Many mathematical models in engineering and science applications are described by non-linear partial differential equations (PDEs) whose solutions exhibit inherently non-linear behavior, including static equilibria, transient steady states, periodic or quasi-periodic time-asymptotic regimes, and chaotic oscillations. It is well-known that non-linear equations can be very sensitive to initial

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conditions and parameters appearing in these equations: a slight perturbation of operating conditions can cause the solution of the PDE to change dramatically. The proper characterization of all such solution states becomes particularly important in non-linear control systems applications in which one may be interested in fine-tuning a system parameter, or input, to yield a particular state or configuration of the governing system. Although investigation of stability and sensitivity of non-linear systems can sometimes be carried out analytically using techniques from non-linear analysis [1, 2], numerical bifurcation techniques are required in general. Packages and tools [3] for performing such bifurcation analyses are available; however, these tools are often too computationally expensive for use in a design or analysis setting.

The cost associated with the analysis of non-linear equations has pushed researchers in mathematics and engineering applications to seek modeling and simulation techniques that retain the essential dynamics of a high-fidelity model but at a much lower computational cost. The basic idea of these ‘reduced order models’ (ROMs) is to use a relatively small number of solutions generated by a high-fidelity simulation to construct a model that is much cheaper computationally and can be run in real or near-real time. A ROM to be used in predictive, real-time applications is desired to have the following properties:

- (i) Stability: the ROM should be constructed such that it can be ensured *a priori* that the discretization does not introduce into the approximation any non-physical numerical instabilities inconsistent with any physical instabilities exhibited by the exact solutions to the equations being solved, and
- (ii) Efficiency: the non-linear terms in the ROM should be handled in a way that does not invalidate the label *reduced* order model.

Many non-linear ROM techniques are derived from the proper orthogonal decomposition (POD)/Galerkin projection approach [4–6]. Non-linear POD/Galerkin ROMs have been constructed in a number of applications. An analytical technique based on the POD method and Galerkin projection was presented for the analysis and characterization of inter-area oscillations in stressed power systems in [7]. Dynamical models for bifurcation analysis and control of self-sustained cavity oscillations, also based on the POD/Galerkin approach, were examined by Rowley *et al.* in [8, 9]. In [10], Bizon *et al.* investigated features and limitations of POD models for different snapshot sampling policies for a tubular reactor with recycle. In [11], Agudelo *et al.* presented an application of positive polynomials to the reduction of the number of temperature constraints of a POD-based predictive controller of a similar tubular reactor.

The aim of the present work is to develop an efficient, asymptotically stable model reduction approach based on the POD/Galerkin projection for non-linear PDEs exhibiting complex non-linear dynamics, such as metastability (stable or unstable fixed points that coalesce or vanish on a long time scale) and periodic, oscillatory regimes (limit cycles). The proposed model reduction technique is based on the ‘continuous projection’ approach: the continuous, governing PDEs are projected onto the basis modes in a continuous inner product, in common with the perspective of [12–17]. This approach is fundamentally different from a popular approach, termed the ‘discrete projection’ approach, in which the semi-discrete representation of the governing equations is projected onto a set of discrete modes in a discrete inner product. The primary advantage of the continuous projection approach is that it allows the use of numerical analysis techniques employed by the spectral methods community [18, 19] to determine, *a priori*, the stability and convergence properties of the ROM. By using these techniques, a ROM based on the continuous projection approach can be derived to possess, by construction, a certain stability guarantee. As shown in [12–15], the stability of the Galerkin projection step of the model reduction procedure can be closely tied to the choice of inner product and the formulation and implementation of the boundary conditions, which are not necessarily inherited from the discretized equation set by a ROM constructed using the continuous Galerkin projection approach. For non-linear equations, the energy method can be applied to the linearized, constant coefficient version of the continuous problem in order to obtain energy inequalities that bound the temporal growth of the solutions to the initial boundary value problem (IBVP) in regions where the exact solutions to these equations are asymptotically stable [19, 20]. This analysis allows one to identify *a priori* if a particular choice of inner product is the ‘correct’ inner product—‘correct’

from the perspective of stability—for a given equation set. A penalty method implementation of the boundary conditions that preserves asymptotic stability of the ROM with boundary treatment—so as to ensure that the boundary condition terms appearing in the ROM do not destabilize the ROM—may be derived as well also using the energy method. Efficiency of the ROM can be maintained via the ‘best points’ interpolation method (BPIM) of Peraire, Nguyen *et al.* [21, 22].

The remainder of this paper is organized as follows. Section 2 describes the proposed non-linear model reduction procedure. The POD/Galerkin approach for model reduction is overviewed in Section 2.1. In Section 2.2, the inefficiency of the direct projection of the non-linear terms in building a non-linear ROM for equations possessing strong non-linearities is exhibited. It is shown how efficiency can be recovered by applying the so-called BPIM of [21, 22]. The penalty method approach to enforcing boundary conditions is outlined in Section 2.3, and a procedure for studying asymptotic stability of a Galerkin-projected system is described in Section 2.4. In Sections 3 and 4, efficient ROMs are developed for the non-linear Allen-Cahn (or ‘bistable’) equation and a convection-diffusion-reaction (CDR) model of a tubular reactor, respectively. For both problems considered, a penalty implementation of the boundary conditions is formulated and proven to be asymptotically stable for specific ranges of the penalty parameters. Numerical experiments illustrate that the proposed POD ROMs developed perform well both without and with interpolation of the non-linear terms: the penalty method is effective in enforcing boundary conditions of the Dirichlet, Neumann, and Robin kind, and the ROMs are able to correctly capture the ‘metastability’ phenomenon exhibited by the solution to the former equation and a stable limit cycle exhibited by the solution to the latter system. It is emphasized that the model reduction approach proposed herein and illustrated on these small-scale benchmarks is extendable to more challenging equations and larger scale problems that arise in various industrial and engineering applications, for example, non-linear conservation laws in the field of computational fluid dynamics [14]. Conclusions are offered in Section 5.

2. CONSTRUCTION AND ANALYSIS OF REDUCED ORDER MODELS FOR NON-LINEAR PARTIAL DIFFERENTIAL EQUATIONS

2.1. Proper orthogonal decomposition/Galerkin approach for model reduction

This section contains a brief overview of the POD/Galerkin method for reducing the order of a complex physical system governed by a general set of PDEs. The approach consists of two steps.

The first step is the calculation of a reduced basis using the POD of an ensemble of realizations from a high-fidelity simulation. Discussed in detail in Lumley [23] and Holmes *et al.* [4], POD is a mathematical procedure that, given an ensemble (or snapshot set) of data, denoted by $\{\mathbf{u}^k(\mathbf{x}) : k = 1, \dots, N\}$, constructs a basis for that ensemble that is optimal in the sense that it describes more energy (on average) of the ensemble than any other linear basis of the same dimension M . It is a well-known result [4, 12, 16, 24] that the solution to this optimization problem reduces to the eigenvalue problem $\mathcal{R}\phi = \lambda\phi$, where $\mathcal{R} \equiv \langle \mathbf{u}^k \otimes \mathbf{u}^k \rangle$ is a self-adjoint and positive semi-definite operator. It can be shown [4, 23] that the set of M eigenfunctions, or POD modes, $\{\phi_i : i = 1, 2, \dots, M\}$ corresponding to the M largest eigenvalues of \mathcal{R} is precisely the set of $\{\phi_i\}$ that solves the aforementioned POD optimization problem. Given this basis, the numerical ROM solution \mathbf{u}_M can be represented as a linear combination of POD modes

$$\mathbf{u}_M(\mathbf{x}, t) = \sum_{j=1}^M a_j(t) \phi_j(\mathbf{x}), \quad (1)$$

where the $a_j(t)$ are the so-called ROM coefficients to be solved for in the ROM.

The second step in constructing a ROM involves projecting the governing system of PDEs onto the POD basis $\{\phi_i\}$ in some appropriate inner product, denoted generically (for now) by (\cdot, \cdot) . In this step, the full-system dynamics are effectively translated to the implied dynamics of the POD

modes. If the governing system of equations for the state variable vector \mathbf{u} has the form

$$\frac{\partial \mathbf{u}}{\partial t} = \mathcal{L}\mathbf{u} + \mathcal{N}_2(\mathbf{u}, \mathbf{u}) + \mathcal{N}_3(\mathbf{u}, \mathbf{u}, \mathbf{u}), \quad (2)$$

where \mathcal{L} is a linear differential operator and \mathcal{N}_2 and \mathcal{N}_3 are (non-linear) quadratic and cubic operators respectively, then the Galerkin projection of (2) onto the POD mode ϕ_j for $j = 1, 2, \dots, M$ is

$$\left(\phi_j, \frac{\partial \mathbf{u}_M}{\partial t} \right) = (\phi_j, \mathcal{L}\mathbf{u}_M) + (\phi_j, \mathcal{N}_2(\mathbf{u}_M, \mathbf{u}_M)) + (\phi_j, \mathcal{N}_3(\mathbf{u}_M, \mathbf{u}_M, \mathbf{u}_M)). \quad (3)$$

Substituting the POD decomposition of \mathbf{u}_M (1) into (3) and applying the orthonormality property of the basis functions ϕ_i in the inner product (\cdot, \cdot) gives a set of time-dependent ordinary differential equations (ODEs) in the modal amplitudes (also referred to as the ROM coefficients) that accurately describes the flow dynamics of the full system of PDEs for some limited set of flow conditions:

$$\begin{aligned} \frac{da_j}{dt} \equiv \dot{a}_j &= \sum_{l=1}^M a_l (\phi_j, \mathcal{L}(\phi_l)) + \sum_{l=1}^M \sum_{m=1}^M a_l a_m (\phi_j, \mathcal{N}_2(\phi_l, \phi_m)) \\ &+ \sum_{l=1}^M \sum_{m=1}^M \sum_{n=1}^M a_l a_m a_n (\phi_j, \mathcal{N}_3(\phi_l, \phi_m, \phi_n)), \end{aligned} \quad (4)$$

for $j = 1, 2, \dots, M$.

The approach described herein is based on a Galerkin projection of the *continuous* governing partial differential equations, in common with the perspective of, for example, [12, 13, 15–17]. This ‘continuous projection’ approach differs from many POD/Galerkin applications, where the semi-discrete representation of the governing equations is projected, and numerical analysis proceeds from the perspective of a dynamical system of ODEs. The continuous projection approach has the advantage that the ROM solution behavior can be examined using methods that have traditionally been used for numerical analysis of spectral approximations to partial differential equations [18, 19], such as the techniques employed herein in studying stability. Because the stability analysis of the ROM can be carried out *a priori* at the level of the *continuous* equations, the ROM can be constructed so that its stability is ensured *a priori*. Unlike in the discrete approach, however, in the continuous approach, boundary condition terms present in the discretized equation set are *not* in general inherited by the ROM and must therefore be implemented separately in the ROM (Section 2.3). It is emphasized that even though a ROM constructed using the discrete projection approach has embedded in it the boundary conditions, many ROMs based on the discrete projection approach are constructed without an *a priori* stability guarantee [25, 26]. These ROMs, although potentially unstable, are nonetheless used in some applications because they can be easier to implement than ROMs constructed using the continuous projection method [12, 25].

For the ROMs developed herein, the standard L^2 inner product is selected for the Galerkin projection step of the model reduction procedure, as the Galerkin projection of the equations considered is asymptotically stable in this inner product (Theorems 3.1.1 and 4.1.1)[‡]. In the implementation, the continuous L^2 inner product (\cdot, \cdot) is approximated by a discrete L^2 inner product:

$$(u, v) \equiv \int_{\Omega} u v d\Omega \approx \sum_{k=0}^N u(x_k) v(x_k), \quad (5)$$

where $x_0, \dots, x_N \in \Omega$ are the spatial discretization points.

[‡]Note that for certain systems, for example, the compressible Euler and Navier–Stokes equations, another inner product may be required to preserve stability of the Galerkin approximation compared with [12–15].

2.2. ‘Best points’ interpolation of non-linear terms in the reduced order model

Consider the general non-linear IBVP

$$\frac{\partial u}{\partial t} + \mathcal{L}u + \mathcal{N}(u) = f, \quad (6)$$

where \mathcal{L} is a linear operator, \mathcal{N} is a non-linear operator, and f is some source depending on space only (not a function of u). Assume without loss of generality that u is a scalar-valued function. Projecting (6) onto the j th POD (or any reduced basis) mode, denoted by ϕ_j for $j = 1, \dots, M$, gives rise to a system of ODEs of the form

$$\dot{\mathbf{a}}_M = \mathbf{F} - \mathbf{L}\mathbf{a}_M - \mathbf{N}(\mathbf{a}_M), \quad (7)$$

where $\mathbf{a}_M^T \equiv (a_1, \dots, a_M)$ and

$$L_{ij} \equiv (\mathcal{L}\phi_j, \phi_i), \quad i, j = 1, \dots, M, \quad (8)$$

$$F_i \equiv (f, \phi_i), \quad i = 1, \dots, M, \quad (9)$$

$$N_i(\mathbf{a}_M) \equiv \left(\mathcal{N} \left(\sum_{k=1}^M a_k \phi_k \right), \phi_i \right), \quad i = 1, \dots, M. \quad (10)$$

The inner products in (10) *cannot* be pre-computed prior to time integration of the ROM system (7) if \mathcal{N} contains a strong, for example, a non-polynomial non-linearity; rather, these inner products would need to be recomputed at each time (or Newton) step of the ROM. This ‘direct’ treatment, or computation, of these inner products can greatly reduce the efficiency of the ROM and motivates the consideration of some alternative way to handle the non-linearity in (6).

To recover efficiency, the ‘best points’ interpolation of [21, 22], a technique based on a coefficient function approximation for the non-linear terms in (6), is employed. The general procedure is outlined below.

Suppose K snapshots have been taken of the unknown field u at K different times (the first step of the POD/Galerkin approach for model reduction outlined in Section 2.1):

$$\mathcal{S}^u \equiv \{\xi_k^u(x) = u_h^k(x) : 1 \leq k \leq K\}. \quad (11)$$

Given this set of snapshots of the primal unknown field u , the following set of snapshots of the non-linear function \mathcal{N} appearing in (6) is constructed:

$$\mathcal{S}^{\mathcal{N}} \equiv \{\xi_k^{\mathcal{N}}(x) = \mathcal{N}(u_h^k(x)) : 1 \leq k \leq K\}. \quad (12)$$

The best approximations of the elements in the snapshot set are now defined as follows:

$$\mathcal{N}_M^*(u_h^k(\cdot)) = \arg \min_{w_M \in \text{span}\{\phi_1^{\mathcal{N}}, \dots, \phi_M^{\mathcal{N}}\}} \|\mathcal{N}(u_h^k(\cdot)) - w_M\|, \quad 1 \leq k \leq K, \quad (13)$$

where the set $\{\phi_m^{\mathcal{N}}\}_{m=1}^M$ is an orthonormal basis for \mathcal{N} and $\|\cdot\|$ denotes the norm induced by the inner product (\cdot, \cdot) in which the POD basis is constructed (in this work, the standard L^2 inner product (5)). Orthonormality of the $\phi_m^{\mathcal{N}}$ in this inner product implies that

$$\mathcal{N}_M^*(u_h^k(x)) = \sum_{m=1}^M \alpha_m^k \phi_m^{\mathcal{N}}(x), \quad 1 \leq k \leq K, \quad (14)$$

where

$$\alpha_m^k = (\phi_m^{\mathcal{N}}, \mathcal{N}(u_h^k(\cdot))), \quad m = 1, \dots, M, 1 \leq k \leq K. \quad (15)$$

The ‘best’ interpolation points [21, 22], denoted by $\{x_m^{bp}\}_{m=1}^M$, are defined as the solution to the following optimization problem:

$$\min_{x_1^{bp}, \dots, x_M^{bp} \in \Omega} \sum_{k=1}^K \left\| \mathcal{N}_M^*(u_h^k(\cdot)) - \sum_{m=1}^M \beta_m^k(x_1^{bp}, \dots, x_M^{bp}) \phi_m^{\mathcal{N}} \right\|^2, \quad (16)$$

$$\sum_{n=1}^M \phi_n^{\mathcal{N}}(x_m^{bp}) \beta_n^k(x_1^{bp}, \dots, x_M^{bp}) = \mathcal{N}(u_h^k(x_m^{bp})), \quad 1 \leq m \leq M, 1 \leq k \leq K,$$

that is, the set of points $\{x_m^{bp}\}_{m=1}^M$ is determined to minimize the average error between the interpolants $\mathcal{N}_M(\cdot)$ and the best approximations $\mathcal{N}_M^*(\cdot)$. Substituting (14) into (16) and invoking the orthonormality of the $\{\phi_m^{\mathcal{N}}\}_{m=1}^M$, one can show that (16) is equivalent to

$$\min_{x_1^{bp}, \dots, x_M^{bp} \in \Omega} \sum_{k=1}^K \sum_{m=1}^M (\alpha_m^k - \beta_m^k(x_1^{bp}, \dots, x_M^{bp}))^2, \quad (17)$$

$$\sum_{n=1}^M \phi_n^{\mathcal{N}}(x_m^{bp}) \beta_n^k(x_1^{bp}, \dots, x_M^{bp}) = \mathcal{N}(u_h^k(x_m^{bp})), \quad 1 \leq m \leq M, 1 \leq k \leq K.$$

The solution to the least squares optimization problem (17) can be found using the Levenberg–Marquardt algorithm and is typically reached in less than fifteen iterations of the algorithm [22].

Given the ‘best points’ for \mathcal{N} , that is, the solutions to (17) (or any set of interpolation points), denoted by $\{x_m^{\mathcal{N}}\}_{m=1}^M$, it is straightforward to apply the interpolation procedure outlined in [21, 22] to the non-linear function $\mathcal{N}(u)$ that appears in (6). The first step is to compute snapshots for the non-linear function \mathcal{N} in (6). From these snapshots, the interpolation points $\{x_m^{\mathcal{N}}\}_{m=1}^M$ are computed following the approach outlined previously (and discussed in detail in Section 2 of [22]). Given $\{x_m^{\mathcal{N}}\}_{m=1}^M$ and $\{\phi_m^{\mathcal{N}}\}_{m=1}^M$, the so-called ‘cardinal functions’, denoted by $\{\psi_m^{\mathcal{N}}\}_{m=1}^M$, are computed by solving the following linear system[§]

$$\phi_M^{\mathcal{N}}(x) = \mathbf{A} \psi_M^{\mathcal{N}}(x), \quad (18)$$

where $\phi_M^{\mathcal{N}}(x) = (\phi_1^{\mathcal{N}}(x), \dots, \phi_M^{\mathcal{N}}(x))^T$, $\psi_M^{\mathcal{N}}(x) = (\psi_1^{\mathcal{N}}(x), \dots, \psi_M^{\mathcal{N}}(x))^T$, and $A_{ij} = \phi_j^{\mathcal{N}}(x_i^{\mathcal{N}})$, with the cardinal functions satisfying $\psi_j^{\mathcal{N}}(x_i) = \delta_{ij}$.

Given the interpolation points $\{x_m^{\mathcal{N}}\}$ and the cardinal functions $\{\psi_m^{\mathcal{N}}\}$, the non-linear function \mathcal{N} is approximated as

$$\mathcal{N}(u) \approx \mathcal{N}_M(u) = \sum_{m=1}^M \mathcal{N}(u(x_m^{\mathcal{N}})) \psi_m^{\mathcal{N}} \in \mathbb{R}, \quad (19)$$

so that

$$\mathcal{N}_M(u) = \sum_{m=1}^M \mathcal{N} \left(\sum_{n=1}^M a_n(t) \phi_n(x_m^{\mathcal{N}}) \right) \psi_m^{\mathcal{N}}, \quad (20)$$

where $\{\phi_m\}_{m=1}^M$ is an orthonormal basis for the primal unknown u computed from the snapshots (11).

The projection of $\mathcal{N}_M(u)$ (20) onto the l th POD mode for u can be written in matrix or vector form. To do this, note that, for a general function $\mathcal{N}_M(u)$ and for $l = 1, \dots, M$:

$$\begin{aligned} (\phi_l, \mathcal{N}_M(u)) &= \left(\phi_l, \sum_{m=1}^M \mathcal{N} \left(\sum_{n=1}^M a_n(t) \phi_n(x_m^{\mathcal{N}}) \right) \psi_m^{\mathcal{N}} \right) \\ &= \sum_{m=1}^M \left[\int_{\Omega} \phi_l \psi_m^{\mathcal{N}} d\Omega \right] \mathcal{N} \left(\sum_{n=1}^M a_n(t) \phi_n(x_m^{\mathcal{N}}) \right). \end{aligned} \quad (21)$$

(21) is a matrix or vector product of the form $\mathbf{G}^{\mathcal{N}} \mathcal{N} \left(\sum_{n=1}^M a_n \phi_n(x_m^{\mathcal{N}}) \right)$ where

$$G_{nm}^{\mathcal{N}} = \int_{\Omega} \phi_n \psi_m^{\mathcal{N}} d\Omega, \quad (22)$$

[§]Note that, for \mathbf{A} to be invertible, the number of interpolation points must be equal to the number of reduced basis modes M . A non-linear least squares optimization problem may be formulated if it is desired to have more interpolation points than modes M , but this latter approach is not considered in the present work.

for $1 \leq m, n \leq M$ (so that $\mathbf{G}^{\mathcal{N}} \in \mathbb{R}^{M \times M}$).

It follows that, with the interpolation procedure described here, the ODE system for the ROM coefficients is not (7) but rather

$$\dot{\mathbf{a}}_M = \mathbf{F} - \mathbf{L}\mathbf{a}_M - \mathbf{G}^{\mathcal{N}} \mathcal{N}(\mathbf{D}^{\mathcal{N}} \mathbf{a}_M), \quad (23)$$

where \mathbf{F} and \mathbf{L} are defined in (9) and (8), respectively; the entries of the matrix $\mathbf{G}^{\mathcal{N}}$ are given by (22) and

$$\mathbf{D}^{\mathcal{N}} \equiv \begin{pmatrix} \phi_1(x_1^{\mathcal{N}}) & \dots & \phi_M(x_1^{\mathcal{N}}) \\ \vdots & \ddots & \vdots \\ \phi_1(x_M^{\mathcal{N}}) & \dots & \phi_M(x_M^{\mathcal{N}}) \end{pmatrix} \in \mathbb{R}^{M \times M}. \quad (24)$$

To clarify the notation in (23), namely what is meant by a function \mathcal{N} of a vector:

$$\mathcal{N}(\mathbf{D}^{\mathcal{N}} \mathbf{a}_M) \equiv \mathcal{N} \begin{pmatrix} \sum_{m=1}^M a_m(t) \phi_m(x_1^{\mathcal{N}}) \\ \vdots \\ \sum_{m=1}^M a_m(t) \phi_m(x_M^{\mathcal{N}}) \end{pmatrix} \equiv \begin{pmatrix} \mathcal{N} \left(\sum_{m=1}^M a_m(t) \phi_m(x_1^{\mathcal{N}}) \right) \\ \vdots \\ \mathcal{N} \left(\sum_{m=1}^M a_m(t) \phi_m(x_M^{\mathcal{N}}) \right) \end{pmatrix} \in \mathbb{R}^M. \quad (25)$$

Once the ROM system (23) is constructed, the ROM is solved by advancing this system forward in time using a standard time-integration scheme (e.g., Euler, Runge–Kutta), or a combination of a time-integration scheme and Newton’s method, if the chosen time-integration scheme is implicit.

Essentially, in the BPIM, recomputation of inner products (projection) of the non-linear terms at each time (or Newton) step is replaced by evaluation of the basis functions at the interpolation points. These interpolation points are pre-computed and much fewer in number than N , the number of spatial grid points. Hence, with interpolation, the cost of each step of the online time-integration stage of the model reduction procedure is of $\mathcal{O}(M)$ —compared without $\mathcal{O}(N)$ for the model reduction procedure without interpolation. Because $M \ll N$ in practice, the savings gained in employing the interpolation can be substantial, especially if the governing equation set possesses a strong (non-polynomial) non-linearity $\mathcal{N}(\mathbf{u})$. The computational complexity of the ‘best points’ interpolation algorithm is discussed in detail in [21, 22].

2.3. Penalty enforcement of the boundary conditions in the reduced order model

In a POD ROM developed using the continuous projection approach [12, 13, 15], the boundary condition terms present in the discretized equation set from which the POD basis is generated are not inherited automatically by the ROM solution. The usual way to enforce boundary conditions in a ROM constructed using the continuous projection approach is through a weak implementation, that is, by applying them directly into the boundary integrals that arise when the operator \mathcal{L} in (2) is projected onto a mode and integrated by parts [12, 13, 15]. It has been argued that this weak implementation of the boundary conditions does not take into account the fact that the equation should be obeyed arbitrarily close to the boundary. Indeed, numerical experiments demonstrate that a weak implementation in which the boundary data are substituted direction into the boundary integrals does not work well for some POD ROMs, particularly ROMs for equations with Robin boundary conditions: the ROM solution may exhibit significant errors near the boundaries, error that can grow in time and ultimately corrupt the solution in the entire domain.

An alternative to a weak enforcement of the boundary conditions is a penalty enforcement of boundary conditions [18, 19, 27]. Formulating a boundary condition using the penalty method amounts to rewriting a boundary value problem as follows:

$$\begin{cases} \mathbf{u}_t = \mathcal{L}\mathbf{u} + \mathcal{N}\mathbf{u} + \mathbf{f}, & \text{in } \Omega \\ \mathbf{B}\mathbf{u} = \mathbf{h}, & \text{on } \partial\Omega \end{cases} \rightarrow \mathbf{u}_t = \mathcal{L}\mathbf{u} + \mathcal{N}\mathbf{u} + \mathbf{f} - \mathbf{\Gamma}(\mathbf{B}\mathbf{u} - \mathbf{h})\delta_{\partial\Omega}, \quad (26)$$

in $\Omega \cup \partial\Omega$. Here, $\mathbf{\Gamma}$ is a diagonal matrix of penalty parameters selected such that stability is preserved, and $\delta_{\partial\Omega}$ is an indicator function marking the boundary $\partial\Omega$:

$$\delta_{\partial\Omega} \equiv \begin{cases} 1, & \text{for } \mathbf{x} \in \partial\Omega \\ 0, & \text{otherwise.} \end{cases} \quad (27)$$

A useful technique for deriving the penalty parameters in $\mathbf{\Gamma}$ such that the Galerkin projection of (26) remains stable is described in [19]. This technique, outlined in Section 2.4, is employed in the analyses performed in Sections 3.1 and 4.1.

2.4. Stability analysis

For ROMs for general non-linear problems such as the ones considered herein, the question of numerical stability can be a complicated one. This is because non-linear equations can support (exhibit) stable as well as unstable, sometimes even chaotic, solutions. A ROM for a non-linear equation or system of equations can only be expected to remain numerically stable in regions where the exact solution to the equation(s) is in a stable state.

As illustrated in [19, 20], linear stability of a non-linear system can be examined for a large class of operators if the solutions are smooth. For such problems, it is sufficient to consider the questions of well-posedness and asymptotic stability for the locally linearized, constant coefficient version of the full non-linear problem. The goal, then, in building a non-linear ROM, is to formulate the discrete problem with boundary conditions such that the Galerkin projection of the equations can be asymptotically stable in a way that is consistent with the asymptotic stability of the governing continuous equations. This is performed through the selection of an appropriate (stability-preserving) inner product for the given equation set and the development of a stability-preserving implementation of the prescribed boundary conditions. Numerical stability of the ROM is studied via the energy method. The key steps involved in using the energy method to build a ROM with an *a priori* stability guarantee for any given equation set are summarized in the succeeding texts:

Step 1

Select an inner product (\cdot, \cdot) to be used in building the ROM, with a corresponding norm $\|\cdot\|$.

Step 2

Determine the stable steady states supported by the governing non-linear system, for example, (26).

Step 3

Linearize the spatial terms that appear in the equation set about a constant state \mathbf{u}_0 at which the solution exhibits stable behavior, that is, linearize about a state \mathbf{u}_0 for which $\Re\{\lambda(\mathbf{J}_0)\} < 0$; where

$$\mathbf{J}_0 \equiv \frac{\partial(\mathcal{L} + \mathcal{N})}{\partial \mathbf{u}} \Big|_{\mathbf{u}=\mathbf{u}_0} . \quad (28)$$

Step 4

Ensure that the rate of change of the localized (frozen coefficient) and linearized system energy, given by

$$\frac{1}{2} \frac{d}{dt} \|\mathbf{u}\|^2 = (\mathbf{J}_0 \mathbf{u} + \mathbf{f}, \mathbf{u}), \quad (29)$$

is non-positive (the system energy is non-increasing[¶])—that is, ensure that the Galerkin projection step of the model reduction without boundary treatment is stable in the chosen inner product.

Step 5

If an energy stability bound of the form (29) cannot be shown, return to Step 1 and select an alternative inner product for the model reduction; otherwise, proceed to Step 6.

[¶]Non-increasing system energy is a sufficient condition for stability of the Galerkin scheme.

Step 6

Derive the penalty parameters (the entries of Γ) such that the rate of change of the localized (frozen coefficient) and linearized system energy with penalty-enforced boundary treatment, given by

$$\frac{1}{2} \frac{d}{dt} \|\mathbf{u}\|^2 = (\mathbf{J}_0 \mathbf{u} + \mathbf{f}, \mathbf{u}) - \Gamma \int_{\partial\Omega} (\mathbf{B}\mathbf{u} - \mathbf{h}) \cdot \mathbf{u} dS, \quad (30)$$

is non-positive (that is, the system energy remains non-increasing following the addition of boundary condition terms).

In the analyses of Sections 3.1 and 4.1, the energy estimate (30) in Step 6 is recast into an algebraic eigenvalue problem, following the procedure of [19].

3. A STABLE PROPER ORTHOGONAL DECOMPOSITION REDUCED ORDER MODEL FOR THE ALLEN–CAHN (OR ‘BISTABLE’) EQUATION

The Allen–Cahn, or ‘bistable’, equation is an example of a semi-linear reaction–diffusion equation. In $(0, T] \times \mathbb{R}^N$, the equation has the form:

$$u_t = \varepsilon \Delta u + f(u), \quad f(u) \equiv u(1 - u^2), \quad (31)$$

where Δ is the usual Laplacian operator and $\varepsilon > 0$ is a parameter, representing diffusivity. First proposed by S. M. Allen and J. W. Cahn in the 1970s as a model for grain boundary motion in crystalline solids [28], Allen–Cahn equations have become a prototype model for isothermal phase transitions. These equations arise in the study of mechanisms of pattern formation for various phenomena, such as phase transition, morphogenesis, population genetics, and chemical reactions.

In the present work, equation (31) in one spatial dimension (1D) is considered:

$$\begin{cases} u_t = \varepsilon u_{xx} + u(1 - u^2), & x \in (-1, 1), \quad t \in (0, T], \\ u(-1, t) = -1, u(1, t) = 1, & t \in (0, T], \\ u(x, 0) = 0.53x - 0.47 \sin\left(\frac{3}{2}\pi x\right), & x \in (-1, 1) \end{cases} \quad (32)$$

The initial condition and the solution to this IBVP are plotted in Figure 1. It is straightforward to find the fixed points of (32), namely by setting $f(u^*) = 0$ and solving for u^* . The equation has three uniform fixed points:

$$u^* = \{-1, 0, 1\}. \quad (33)$$

Stability of these states can be studied by computing the Jacobian

$$J(u) \equiv \frac{\partial f}{\partial u} = 1 - 3u^2, \quad (34)$$

and checking its sign when evaluated at each of the steady states. This analysis leads to the conclusion that the middle state is unstable, but the states $u^* = \pm 1$ are attracting. The solutions to equation (32) exhibit a phenomenon known as ‘metastability’, characterized by relative flatness of the solution close to the stable states, separated by interfaces that may coalesce or vanish on a long time scale [29] (Figure 1(b)).

3.1. Stability-preserving penalty formulation of boundary conditions for the Allen–Cahn Equation

In this section, a stability-preserving penalty enforcement of the boundary conditions for the Allen–Cahn equation (32) is formulated. The first step is to rewrite (32) with a penalty method formulation of the boundary conditions:

$$\begin{cases} u_t = \varepsilon u_{xx} + u(1 - u^2) - \tau_1[u(-1, t) + 1] - \tau_2[u(1, t) - 1], & x \in (-1, 1), \quad t \in (0, T], \\ u(x, 0) = 0.53x - 0.47 \sin\left(\frac{3}{2}\pi x\right), & x \in (-1, 1), \end{cases} \quad (35)$$

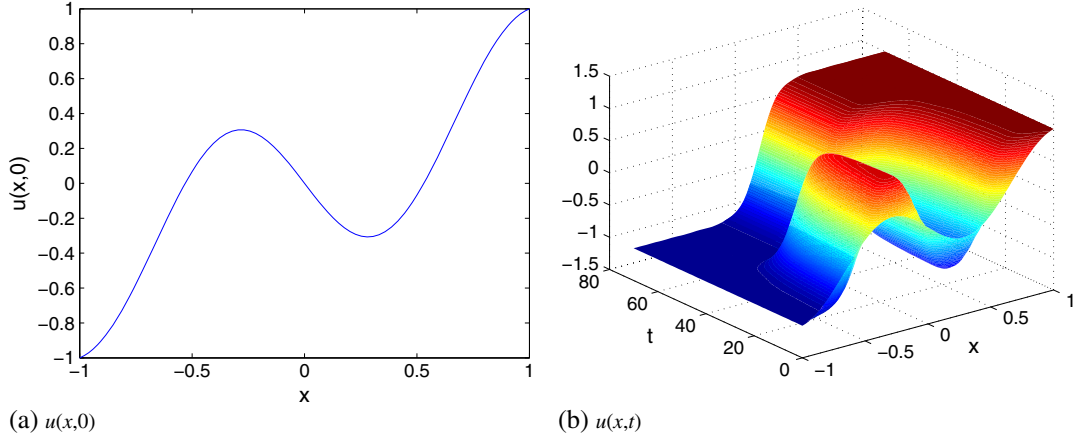


Figure 1. Plots of initial condition (a) $u(x, 0)$ and solution to the Allen–Cahn initial boundary value problem (32) (b) $u(x, t)$.

for some penalty parameters $\tau_1, \tau_2 \in \mathbb{R}$, to be determined such that the Galerkin projection of (35) in the L^2 inner product is linearly stable (Theorem 3.1.1).

Theorem 3.1.1

Let $u_0 \in \mathbb{R}$ be a stable steady state for the 1D Allen–Cahn equation (31) so that $J(u_0) \leq 0$ (34). Then, the Galerkin projection of the IBVP (35) with a penalty enforcement of the boundary conditions is asymptotically stable about u_0 if

$$\tau_1, \tau_2 \geq \underbrace{1 - 3u_0^2}_{J(u_0)} + \frac{1}{4}\varepsilon. \quad (36)$$

Proof

The first step in the analysis is to linearize the function $f(u)$ in (31) about u_0 :

$$u_t \approx \varepsilon u_{xx} + f(u_0) + J(u_0)(u - u_0) = \varepsilon u_{xx} + (1 - 3u_0^2)u + k, \quad (37)$$

where $k \equiv -(1 - 3u_0^2)u_0$ is a constant depending on u_0 . According to the definition of stability (see Definition 2.11 in [30]), it is sufficient to consider the homogeneous version of (37) in studying stability. Therefore, the constant k is neglected from this point forward, and the homogeneous analogs of the boundary conditions in (35) are considered. Then

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|u\|^2 &= \varepsilon (u_{xx}, u) + (1 - 3u_0^2)(u, u) - \tau_1 u^2(-1, t) - \tau_2 u^2(1, t) \\ &= -\varepsilon \|u_x\|^2 + \varepsilon u(1, t) u_x(1, t) - \varepsilon u(-1, t) u_x(-1, t) \\ &\quad + (1 - 3u_0^2) \|u\|^2 - \tau_1 u^2(-1, t) - \tau_2 u^2(1, t) \\ &\leq -\varepsilon u_x^2(1, t) - \varepsilon u_x^2(-1, t) + \varepsilon u(1, t) u_x(1, t) - \varepsilon u(-1, t) u_x(-1, t) \\ &\quad + (1 - 3u_0^2) u^2(1, t) + (1 - 3u_0^2) u^2(-1, t) - \tau_1 u^2(-1, t) - \tau_2 u^2(1, t) \\ &= (1 - 3u_0^2 - \tau_2) u^2(1, t) + \varepsilon u(1, t) u_x(1, t) - \varepsilon u_x^2(1, t) + (1 - 3u_0^2 - \tau_1) u^2(-1, t) \\ &\quad - \varepsilon u(-1, t) u_x(-1, t) - \varepsilon u_x^2(-1, t) \\ &= \mathbf{u}_R^T \mathbf{H}_R \mathbf{u}_R + \mathbf{u}_L^T \mathbf{H}_L \mathbf{u}_L, \end{aligned} \quad (38)$$

where

$$\mathbf{H}_R = \frac{1}{2} \begin{pmatrix} 2 - 6u_0^2 - 2\tau_2 & \varepsilon \\ \varepsilon & -2\varepsilon \end{pmatrix}, \quad \mathbf{H}_L = \frac{1}{2} \begin{pmatrix} 2 - 6u_0^2 - 2\tau_1 & -\varepsilon \\ -\varepsilon & -2\varepsilon \end{pmatrix}, \quad (39)$$

and

$$\mathbf{u}_R \equiv \begin{pmatrix} u(1, t) \\ u_x(1, t) \end{pmatrix}, \quad \mathbf{u}_L \equiv \begin{pmatrix} u(-1, t) \\ u_x(-1, t) \end{pmatrix}. \quad (40)$$

In going from step 2 to step 3 of (38), the norm identity or inequality

$$-||u_x|| = -\sum_{j=0}^N u_x^2(x_j) = -u_x^2(-1, t) - u_x^2(1, t) - \sum_{j=1}^{N-1} u_x^2(x_j) \leq -u_x^2(-1, t) - u_x^2(1, t), \quad (41)$$

has been employed (and similarly for $||u||$), where $x_j \in (-1, 1)$ are the spatial discretization points employed in the numerical scheme. The fact that, by assumption, $J(u_0) = 1 - 3u_0^2 \leq 0$ (u_0 is a point at which the system is asymptotically stable), has been employed as well.

The eigenvalues of \mathbf{H}_R are

$$\lambda_{\pm}(\mathbf{H}_R) = \frac{1 - 3u_0^2 - \tau_2 - \varepsilon \pm \sqrt{1 - 6u_0^2 - 2\tau_2 + 2\varepsilon + 9u_0^4 + 6u_0^2\tau_2 - 6u_0^2\varepsilon + \tau_2^2 - 2\tau_2\varepsilon + 2\varepsilon^2}}{2}. \quad (42)$$

Some algebra reveals that these eigenvalues are non-positive if

$$\tau_2 \geq 1 - 3u_0^2 + \frac{1}{4}\varepsilon. \quad (43)$$

By inspection, the matrix \mathbf{H}_L in (39) has the same trace and determinant as the matrix \mathbf{H}_R . It follows that the two matrices have the same eigenvalues. Thus, the condition on τ_1 is the same as the condition on τ_2 , namely (43). \square

To obtain an estimate of what values τ_1 and τ_2 to employ in practice, it is sensible for this example to linearize J about one of the stable fixed points or steady states, namely $u^* = \pm 1$. For these points,

$$J(\pm 1) = -2, \quad (44)$$

so that (36) reduces to the bound

$$\tau_1 \tau_2 \geq -2 + \frac{1}{4}\varepsilon. \quad (45)$$

3.2. Implementation of the Allen–Cahn reduced order model

The implementation of the Galerkin projection step of the model reduction procedure for the Allen–Cahn IBVP with a penalty enforcement of the boundary conditions (35) is now outlined. Projecting the first line of this IBVP onto the j th POD mode and invoking the orthonormality of the modes give rise to the following system for the time-dependent ROM coefficient $a_j(t)$ (following an integration by parts on the diffusion term):

$$\begin{aligned} \dot{a}_j = \sum_{k=1}^M a_j & \left[-\varepsilon(\phi_{k,x}, \phi_{j,x}) + (\phi_k, \phi_j) + \varepsilon[\phi_{k,x}(1)\phi_j(1) - \phi_{k,x}(-1)\phi_j(-1)] \right. \\ & \left. - \tau_1 \phi_k(-1)\phi_j(-1) - \tau_2 \phi_k(1)\phi_j(1) \right] - \tau_1 \phi_j(-1) + \tau_2 \phi_j(1) + (\mathcal{N}(u_M), \phi_j), \end{aligned} \quad (46)$$

for $j = 1, \dots, M$, where

$$\mathcal{N}(u_M) \equiv -u_M^3, \quad (47)$$

and $u_M \equiv \sum_{k=1}^M a_k(t)\phi_k(x)$.

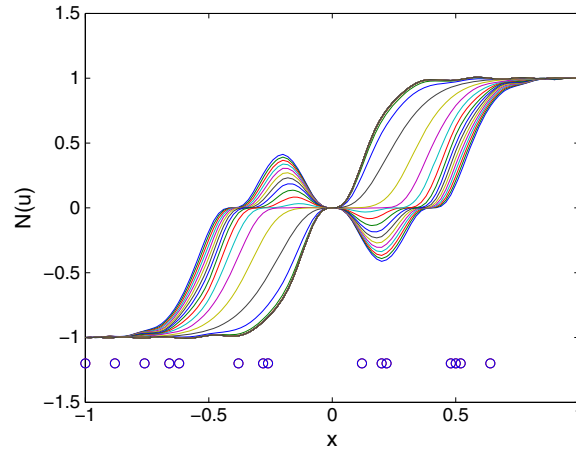


Figure 2. $\mathcal{N}(u)$ (47) (solid lines) and interpolation points (circles) for the Allen–Cahn equation (proper orthogonal decomposition basis, $M = 15$).

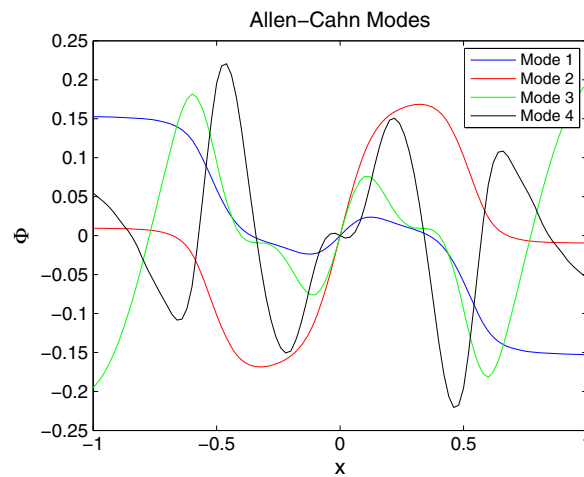


Figure 3. Proper orthogonal decomposition modes for the Allen–Cahn equation.

Figure 2 shows the computed ‘best points’ for a POD basis with $M = 15$ (shown in circles) compared with the non-linear function $\mathcal{N}(u)$ (47). Each curve plotted in this figure shows $\mathcal{N}(u)$ at a different time t .

3.3. Numerical results for the Allen–Cahn initial boundary value problem

A high-fidelity solution from which snapshots were taken to build the ROM was computed using a Chebyshev collocation spectral method in space and a fourth-order Runge–Kutta scheme in time. $N = 101$ spatial discretization points were used with $\Delta x = 0.02$. The POD basis for the ROM was computed from a total of $K = 40$ snapshots. Twenty of these were snapshots of the solution to (32) with $\varepsilon = 0.02$; the remaining twenty were snapshots of the solution to (32) with $\varepsilon = 0.005$. For each value of the diffusivity, the solution snapshots were saved every $\Delta t_{\text{snap}} = 1$ time step until time $T = 20$. Figure 3 shows the first four POD modes computed for this problem. It is evident that these modes do not satisfy the Dirichlet boundary conditions at $x = \pm 1$.

In studying the performance of the proposed model reduction procedure, the predictive capability of the ROM is of interest. To this effect, a ROM for (32) with $\varepsilon = 0.001$ is constructed and evaluated. Note that this value of the diffusivity differs from the values of the diffusivity selected in building the reduced basis modes employed in the ROM. Results (ROM solutions versus high-

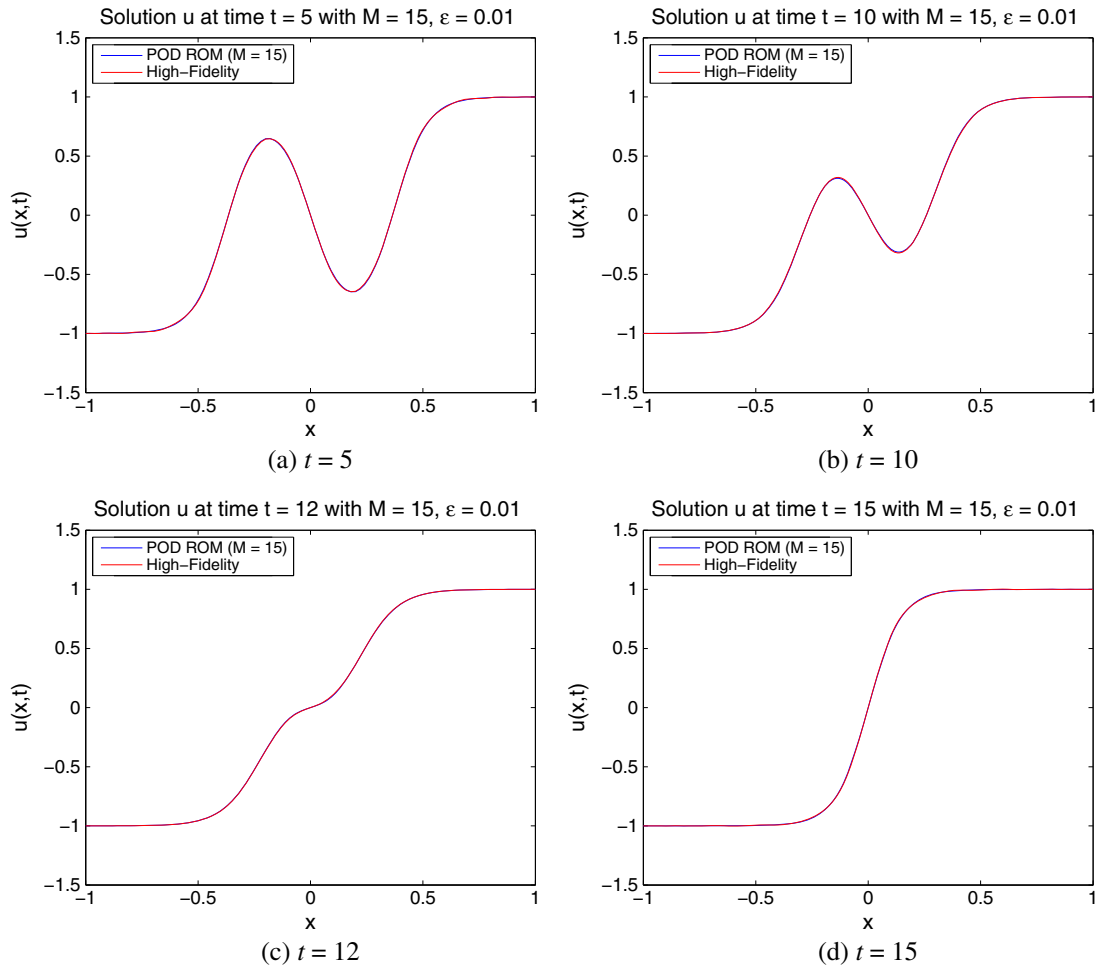


Figure 4. Reduced order model (ROM) solutions to the Allen–Cahn equation with $M = 15$ proper orthogonal decomposition modes, $\varepsilon = 0.01$, $\tau_1 = \tau_2 = 100$ (with interpolation). (a) $t = 5$; (b) $t = 10$; (c) $t = 12$; and (d) $t = 15$.

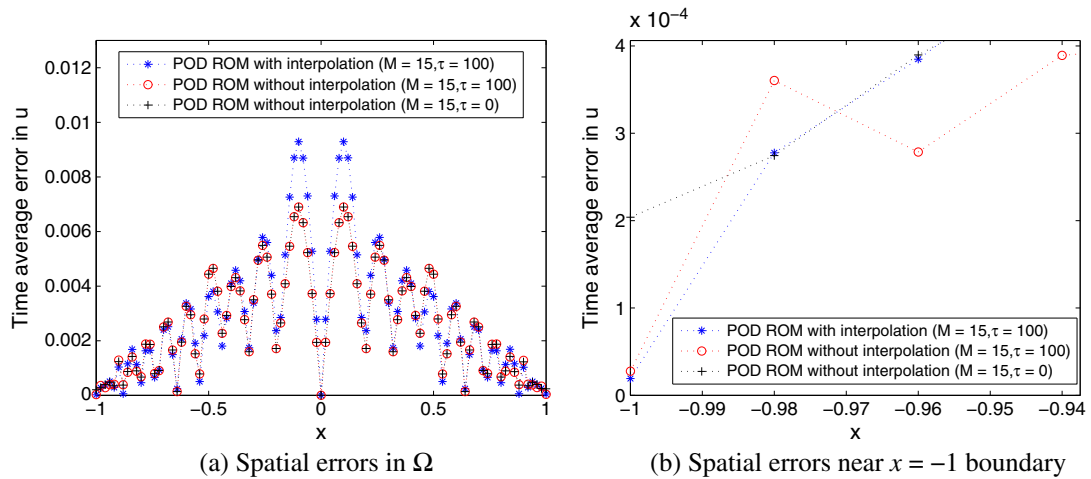


Figure 5. Time-average errors for the reduced order model solutions to the Allen–Cahn equation with $M = 15$ proper orthogonal decomposition modes, $\varepsilon = 0.01$, different $\tau \equiv \tau_1 = \tau_2$. (a) Spatial errors in Ω and (b) Spatial errors near $x = -1$ boundary.

fidelity solutions at different times t) for values of $\tau \equiv \tau_1 = \tau_2$ selected within the stable range derived in Theorem 3.1.1 are shown in Figure 4. For $M \geq 10$, the ROM solution with interpolation looks indistinguishable from the ROM solution without interpolation. Figure 5 shows time-average errors in the ROM solution relative to the CFD solution at each grid point $x_j \in (-1, 1)$ with τ selected within the stable range (45). The time-average error is defined as

$$\mathcal{E} \equiv \frac{1}{T} \sum_{t_{\text{snap}} \leq T} |u_{\text{ROM}}(x_j, t_{\text{snap}}) - u_{\text{ref}}(x_j, t_{\text{snap}})|, \quad (48)$$

where the t_{snap} are the times at which the snapshots were taken, u_{ROM} is the ROM solution, and u_{ref} is a high-fidelity reference solution, employed in the error analysis in place of the exact solution, as the latter is unavailable analytically for this problem. The accuracy of the ROM with interpolation is comparable to the accuracy of the ROM with a direct treatment of the non-linear term (47) at most of the grid points. Figure 5 (b) shows a close up of the errors near the left boundary, $x = -1$. Although the ROM remains stable for $\tau = 0$ (a value within the stability region (45)), it is evident from this plot that the Dirichlet boundary condition at this boundary is being enforced with some error. This situation improves by selecting a larger τ . The time-average error (48) at the point $x = -1$ is plotted as a function of τ for $\tau \in [0, 100]$ in Figure 6. The reader may observe by examining this figure the convergence of the solution at the left boundary with increasing penalty parameter.

As expected, the ROM goes unstable if τ is selected outside the stability range derived in Theorem 3.1.1 (Figure 7). In this ROM, the non-linear term is handled directly. Therefore the instability cannot be attributed to a poor set of interpolation points.

4. A STABLE PROPER ORTHOGONAL DECOMPOSITION REDUCED ORDER MODEL FOR A TUBULAR REACTOR WITH OSCILLATORY REGIMES

In this section, a ROM for a non-linear system exhibiting more complex non-linear dynamics than the Allen–Cahn equation considered in Section 3, namely oscillatory regimes, is developed. The mathematical model is that of a one-dimensional (1D) non-adiabatic tubular reactor, represented by a non-linear CDR system with a single $A \rightarrow B$ reaction [31]. In dimensionless form, the governing equations, describing the conservation of reactant A and energy for the non-adiabatic tubular reactor

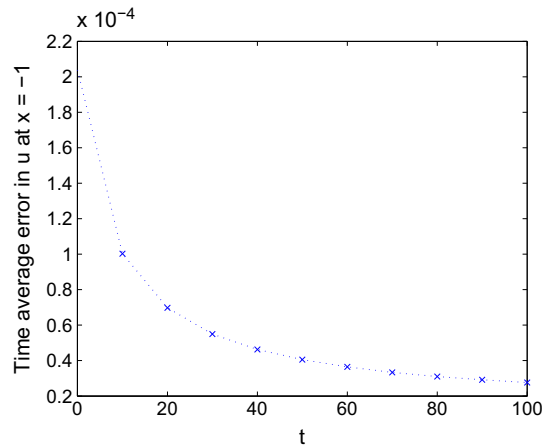


Figure 6. Time-average errors for the reduced order model solutions to the Allen–Cahn equation with $M = 15$ proper orthogonal decomposition modes, $\varepsilon = 0.01$ at the left boundary $x = -1$ as a function of $\tau \equiv \tau_1 = \tau_2$.

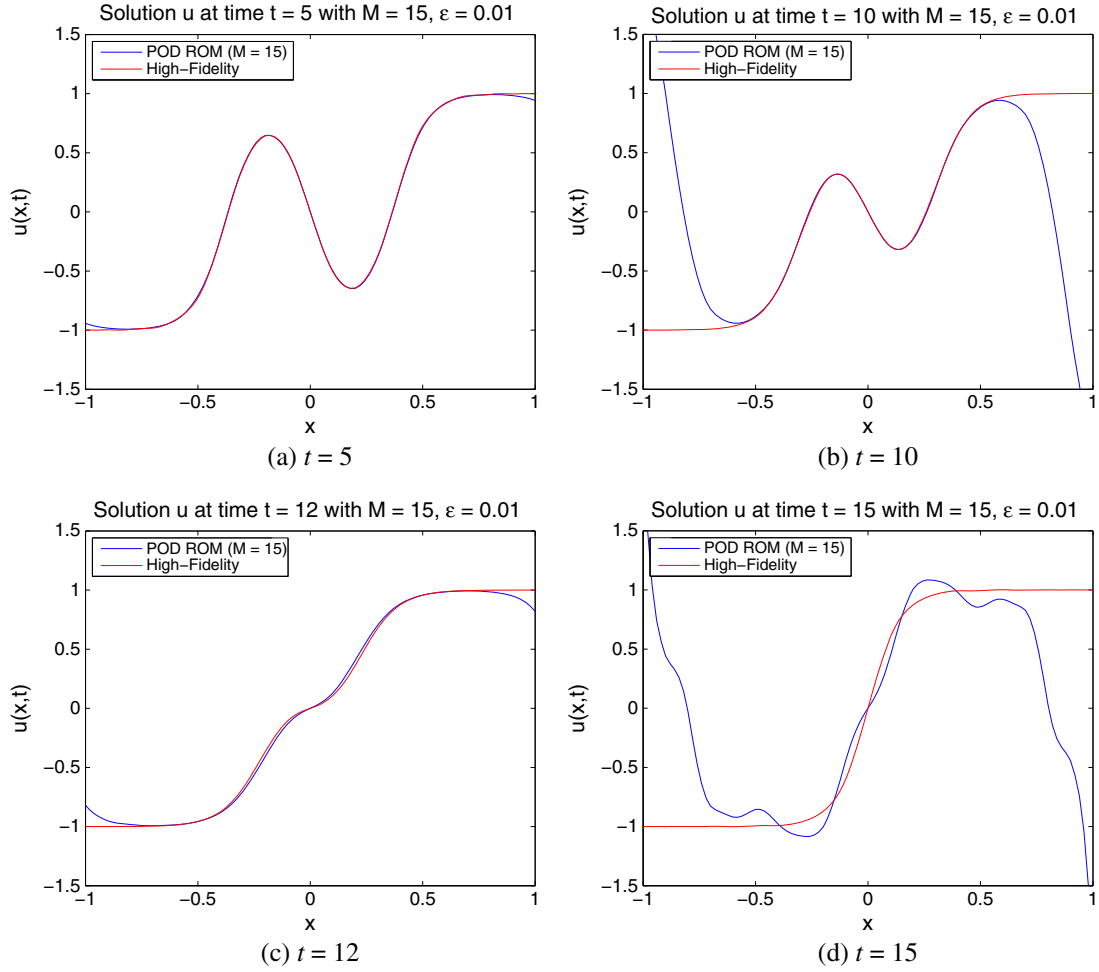


Figure 7. Reduced order model solutions to the Allen–Cahn equation with $M = 15$ proper orthogonal decomposition modes, $\varepsilon = 0.01$, $\tau_1 = \tau_2 = -10$ (no interpolation). (a) $t = 5$; (b) $t = 10$; (c) $t = 12$; and (d) $t = 15$.

with mixing, are^{ll}

$$\begin{aligned} \frac{\partial y}{\partial t} &= \frac{1}{Pe_M} \frac{\partial^2 y}{\partial x^2} - \frac{\partial y}{\partial x} - D(y+1)e^{\frac{\gamma\theta}{\theta+1}}, & x \in (0, 1), \quad t \in [0, T], \\ \frac{\partial \theta}{\partial t} &= \frac{1}{Pe_H} \frac{\partial^2 \theta}{\partial x^2} - \frac{\partial \theta}{\partial x} - \beta(\theta+1-\theta_0) + BD(y+1)e^{\frac{\gamma\theta}{\theta+1}}, & x \in (0, 1), \quad t \in [0, T], \end{aligned} \quad (49)$$

for $\theta_0 \in \mathbb{R}$, $Pe_M, Pe_H > 0$, subject to boundary conditions

$$\begin{cases} \frac{\partial y}{\partial x}|_{x=0} = Pe_M y|_{x=0}, & t \in (0, T], \\ \frac{\partial \theta}{\partial x}|_{x=0} = Pe_H \theta|_{x=0}, & t \in (0, T], \end{cases} \quad (50)$$

^{ll}Note that the equations (49)–(52) are exactly the equations considered in [31] but with the transformation $y \leftarrow y + 1$, $\theta \leftarrow \theta + 1$.

$$\begin{cases} \frac{\partial y}{\partial x}|_{x=1} = 0, & t \in (0, T], \\ \frac{\partial \theta}{\partial t}|_{x=1} = 0, & t \in (0, T], \end{cases} \quad (51)$$

and initial conditions

$$y|_{t=0} = y_{in}, \quad \theta|_{t=0} = \theta_{in}, \quad x \in (0, 1). \quad (52)$$

Here, y is the dimensionless concentration, θ is the dimensionless temperature, x is the dimensionless axial distance, t is the dimensionless time, β is the dimensionless heat transfer coefficient, γ is the dimensionless activation energy, D is the Damköhler number, B is the dimensionless heat of reaction, and Pe_M and Pe_H are the Péclet numbers for mass and heat transfer, respectively. The boundary conditions enforced are of a mixed form: Neumann at the right boundary $x = 1$ (51) and Robin at the left boundary $x = 0$ (50).

It is convenient to write (49)–(52) in vector form, as follows:

$$\begin{cases} \frac{\partial \mathbf{u}}{\partial t} = \mathbf{P} \frac{\partial^2 \mathbf{u}}{\partial x^2} - \frac{\partial \mathbf{u}}{\partial x} - \mathbf{B}(\mathbf{u} + \mathbf{e}_2 - \mathbf{u}_0) - \mathbf{C}\mathcal{N}(\mathbf{u}), & x \in (0, 1), \quad t \in (0, T], \\ \mathbf{P} \frac{\partial \mathbf{u}}{\partial x}|_{x=0} = \mathbf{u}|_{x=0}, & t \in (0, T] \\ \frac{\partial \mathbf{u}}{\partial x}|_{x=1} = \mathbf{0}, & t \in (0, T], \\ \mathbf{u}(x, 0) = \mathbf{u}_{in}, & x \in (0, 1), \end{cases} \quad (53)$$

where, for $y_0 \in \mathbb{R}$,

$$\mathbf{u} \equiv \begin{pmatrix} y \\ \theta \end{pmatrix}, \quad \mathbf{u}_0 \equiv \begin{pmatrix} y_0 \\ \theta_0 \end{pmatrix}, \quad \mathbf{u}_{in} \equiv \begin{pmatrix} y_{in} \\ \theta_{in} \end{pmatrix}, \quad (54)$$

$$\mathbf{P} \equiv \begin{pmatrix} Pe_M^{-1} & 0 \\ 0 & Pe_H^{-1} \end{pmatrix}, \quad \mathbf{B} \equiv \begin{pmatrix} 0 & 0 \\ 0 & \beta \end{pmatrix}, \quad \mathbf{C} \equiv \begin{pmatrix} D \\ -BD \end{pmatrix}, \quad \mathbf{e}_2 \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (55)$$

and

$$\mathcal{N}(\mathbf{u}) \equiv (y + 1)e^{\frac{\gamma\theta}{\theta+1}} \in \mathbb{R}. \quad (56)$$

The fixed points of (49) are the zeros of the non-linear function (56). By inspection, it is straightforward to see that $(y^*, \theta^*) = (-1, k)$, for any $k \in \mathbb{R}$ is a family of fixed points.

Let

$$\mathbf{f}(y, \theta) \equiv \begin{pmatrix} -D(y + 1)e^{\frac{\gamma\theta}{\theta+1}} \\ -\beta\theta + BD(y + 1)e^{\frac{\gamma\theta}{\theta+1}} \end{pmatrix} = -\mathbf{B}\mathbf{u} - \mathbf{C}\mathcal{N}(\mathbf{u}). \quad (57)$$

The Jacobian of (57) is given by

$$\mathbf{J}(\mathbf{u}) \equiv \frac{\partial \mathbf{f}}{\partial \mathbf{u}} = \begin{pmatrix} -D & -D\gamma h(\mathbf{u}) \\ BD & -\beta + BD\gamma h(\mathbf{u}) \end{pmatrix} g(\theta), \quad (58)$$

where

$$h(\mathbf{u}) \equiv \frac{y + 1}{(\theta + 1)^2}, \quad g(\theta) \equiv e^{\frac{\gamma\theta}{\theta+1}}. \quad (59)$$

The eigenvalues of $\mathbf{J}(\mathbf{u})$ are

$$\begin{aligned} \lambda_{1,2} = \frac{g(\theta)}{2} & \left(BD\gamma h(\mathbf{u}) - D - \beta \right. \\ & \left. \pm \sqrt{D^2 - 2D\beta - 2D^2\gamma h(\mathbf{u})B + \beta^2 - 2\beta BD\gamma h(\mathbf{u}) + B^2 D^2 \gamma^2 h^2(\mathbf{u})} \right). \end{aligned} \quad (60)$$

It is apparent (because $\mathbf{J}(-1, k)$ is lower triangular) that $\lambda\{\mathbf{J}(-1, k)\} = -De^{\frac{\gamma k}{k+1}}, -\beta e^{\frac{\gamma k}{k+1}}$, both of which are necessarily negative, meaning $(y^*, \theta^*) = (-1, k)$, for $k \in \mathbb{R}$ defines a region of stable solutions.

As it turns out, the dynamics of the non-linear problem (49) are more complex than those of the Allen–Cahn equation considered previously. These behaviors are studied using numerical bifurcation techniques [31], which reveal periodic solutions possessing Hopf bifurcations and multiplicity patterns exhibiting from one to seven steady states. The existence of stable oscillatory solutions as a function of the Damköhler number D when $Pe_M = Pe_H = 5$, $B = 0.50$, $\gamma = 25$, $\beta = 2.5$, and $\theta_0 = 1$ can be shown. In particular, there is a stable orbit that bifurcates into a limit cycle at the lower Hopf point, $D = 0.165$ (Figure 13).

4.1. Stability-preserving penalty formulation of boundary conditions for the tubular reactor problem

The penalty formulation of (49) with boundary conditions (50) and (51) is

$$\frac{\partial \mathbf{u}}{\partial t} = \mathbf{P} \frac{\partial^2 \mathbf{u}}{\partial x^2} - \frac{\partial \mathbf{u}}{\partial x} - \mathbf{B}(\mathbf{u} + \mathbf{e}_2 - \mathbf{u}_0) - \mathbf{C}\mathcal{N}(\mathbf{u}) - \tau_1 \left(\mathbf{u}|_{x=0} - \mathbf{P} \frac{\partial \mathbf{u}}{\partial x} \Big|_{x=0} \right) - \tau_2 \frac{\partial \mathbf{u}}{\partial x} \Big|_{x=1}, \quad (61)$$

for some penalty parameters $\tau_1, \tau_2 \in \mathbb{R}$ (to be determined).

As with the Allen–Cahn equation, linear stability of the penalty formulation of the boundary conditions for the CDR tubular reactor problem (61) is studied following a linearization of the non-linear function that appears in this system. Suppose that \mathbf{f} (57) has been linearized about some stable state \mathbf{u}_0 :

$$\mathbf{f}(\mathbf{u}) \approx \mathbf{f}(\mathbf{u}_0) + \mathbf{J}(\mathbf{u}_0)(\mathbf{u} - \mathbf{u}_0) = \mathbf{J}(\mathbf{u}_0)\mathbf{u} + \mathbf{c}, \quad (62)$$

for some constant vector $\mathbf{c} \in \mathbb{R}^2$ depending on \mathbf{u}_0 . Introducing the shorthand $\mathbf{J}_0 \equiv \mathbf{J}(\mathbf{u}_0)$, it follows that the linearized variant of (61), written in vector form is

$$\mathbf{u}_t = \mathbf{P}\mathbf{u}_{xx} - \mathbf{u}_x + \mathbf{J}_0\mathbf{u} + \mathbf{c} - \tau_1 [\mathbf{u}(0, t) - \mathbf{P}\mathbf{u}_x(0, t)] - \tau_2 \mathbf{u}_x(1, t), \quad (63)$$

where \mathbf{P} is given by (55).

An energy stability analysis applied to (63) gives bounds on the penalty parameters τ_1 and τ_2 such that the Galerkin projection of these equations in the L^2 inner product is asymptotically stable about a stable state \mathbf{u}_0 (Theorem 4.1.1).

Theorem 4.1.1

Let $\mathbf{u}_0^T \equiv (y_0, \theta_0) \in \mathbb{R}^2$ be a stable point for the CDR tubular reactor system (49) so that $\Re\{\lambda(\mathbf{J}(\mathbf{u}_0))\} \leq 0$. Then, the Galerkin projection of the IBVP with a penalty enforcement of the boundary conditions is asymptotically stable about \mathbf{u}_0 if

$$\begin{aligned} & \max_{i=1,2} \left\{ 0, 2Pe + 1 - \sqrt{4Pe^2 + 2Pe - 4Pe\lambda_0^i} \right\} \\ & \leq \tau_1 \leq \min_{i=1,2} \left\{ 2Pe + 1 + \sqrt{4Pe^2 + 2Pe - 4Pe\lambda_0^i} \right\}, \end{aligned} \quad (64)$$

$$\max_{i=1,2} \left\{ \frac{1 - \sqrt{2Pe - 4Pe\lambda_0^i}}{Pe} \right\} \leq \tau_2 \leq \min_{i=1,2} \left\{ \frac{1 + \sqrt{2Pe - 4Pe\lambda_0^i}}{Pe} \right\}, \quad (65)$$

where λ_0^i , $i = 1, 2$ are the eigenvalues of $\mathbf{J}_0 \equiv \mathbf{J}(\mathbf{u}_0)$ (58) and $Pe = \min\{Pe_M, Pe_H\}^{**}$.

**Note that the range for τ_2 (65) is necessarily defined as $\lambda_0^i < 0$ and $Pe > 0$.

Proof

Let $Pe \equiv \min\{Pe_M, Pe_H\}$ and assume $Pe_M = Pe_H > 0$, $\tau_1 \geq 0$. Then,

$$\mathbf{u}_t \leq Pe^{-1} \mathbf{u}_{xx} - \mathbf{u}_x + \mathbf{J}_0 \mathbf{u} + \mathbf{c} - \tau_1 [\mathbf{u}(0, t) - Pe^{-1} \mathbf{u}_x(0, t)] - \tau_2 \mathbf{u}_x(1, t). \quad (66)$$

The two equations in (66) are coupled by the Jacobian matrix \mathbf{J}_0 . These equations can be decoupled by diagonalizing \mathbf{J}_0 :

$$\mathbf{J}_0 = \mathbf{S}_0 \mathbf{\Lambda}_0 \mathbf{S}_0^{-1}, \quad (67)$$

where

$$\mathbf{\Lambda}_0 \equiv \begin{pmatrix} \lambda_0^1 & 0 \\ 0 & \lambda_0^2 \end{pmatrix} \quad (68)$$

is a diagonal matrix containing the eigenvalues of \mathbf{J}_0 and \mathbf{S}_0 is a matrix with columns spanned by the normalized eigenvectors of \mathbf{J}_0 . Let

$$\mathbf{v} \equiv \mathbf{S}_0^{-1} \mathbf{u}. \quad (69)$$

In these variables, (66) becomes

$$\mathbf{v}_t \leq Pe^{-1} \mathbf{v}_{xx} - \mathbf{v}_x + \mathbf{\Lambda}_0 \mathbf{v} + \mathbf{S}_0^{-1} \mathbf{c} - \tau_1 [\mathbf{v}(0, t) - Pe^{-1} \mathbf{v}_x(0, t)] - \tau_2 \mathbf{v}_x(1, t) \quad (70)$$

or, equivalently,

$$\begin{cases} v_{1,t} \leq Pe^{-1} v_{1,xx} - v_{1,x} + \lambda_0^1 v_1 - \tau_1 [v_1(0, t) - Pe^{-1} v_{1,x}(0, t)] - \tau_2 v_{1,x}(1, t), \\ v_{2,t} \leq Pe^{-1} v_{2,xx} - v_{2,x} + \lambda_0^2 v_2 - \tau_1 [v_2(0, t) - Pe^{-1} v_{2,x}(0, t)] - \tau_2 v_{2,x}(1, t), \end{cases} \quad (71)$$

where $\mathbf{v}^T \equiv (v_1, v_2)$.

Each of the components in (71) is considered one at a time. Setting $\mathbf{c} = \mathbf{0}$ and using the identity $(v_{1,x}, v) \equiv \frac{1}{2} \int_{\Omega} (v^2)_x dx$ as well as (41),

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|v_1\|^2 &\leq Pe^{-1} (v_{1,xx}, v_1) - (v_{1,x}, v_1) + \lambda_0^1 (v_1, v_1) - \tau_1 (v_1(0, t) \\ &\quad - Pe^{-1} v_{1,x}(0, t)) v_1(0, t) - \tau_2 v_{1,x}(1, t) v_1(1, t) \\ &= -Pe^{-1} \|v_{1,x}\|^2 + Pe^{-1} v_{1,x}(1, t) v_1(1, t) - Pe^{-1} v_{1,x}(0, t) v_1(0, t) - \frac{1}{2} v_1^2(1, t) \\ &\quad + \frac{1}{2} v_1^2(0, t) + \lambda_0^1 \|v_1\|^2 - \tau_1 v_1^2(0, t) + \tau_1 Pe^{-1} v_{1,x}(0, t) v_1(0, t) - \tau_2 v_{1,x}(1, t) v_1(1, t) \\ &\leq -Pe^{-1} v_{1,x}^2(0, t) - Pe^{-1} v_{1,x}^2(1, t) + Pe^{-1} v_{1,x}(1, t) v_1(1, t) - Pe^{-1} v_{1,x}(0, t) v_1(0, t) \\ &\quad - \frac{1}{2} v_1^2(1, t) + \frac{1}{2} v_1^2(0, t) + \lambda_0^1 v_1^2(0, t) + \lambda_0^1 v_1^2(1, t) - \tau_1 v_1^2(0, t) \\ &\quad + \tau_1 Pe^{-1} v_{1,x}(0, t) v_1(0, t) - \tau_2 v_{1,x}(1, t) v_1(1, t) \\ &= \left(\frac{1}{2} + \lambda_0^1 - \tau_1 \right) v_1^2(0, t) + (\tau_1 Pe^{-1} - Pe^{-1}) v_{1,x}(0, t) v_1(0, t) - Pe^{-1} v_{1,x}^2(0, t) \\ &\quad + \left(-\frac{1}{2} + \lambda_0^1 \right) v_1^2(1, t) + (Pe^{-1} - \tau_2) v_{1,x}(1, t) v_1(1, t) - Pe^{-1} v_{1,x}^2(1, t) \\ &= \mathbf{v}_{1L}^T \mathbf{H}_{1L} \mathbf{v}_{1L} + \mathbf{v}_{1R}^T \mathbf{H}_{1R} \mathbf{v}_{1R}, \end{aligned} \quad (72)$$

where

$$\mathbf{H}_{1L} \equiv \frac{1}{2Pe} \begin{pmatrix} Pe(1 + 2\lambda_0^1 - 2\tau_1) & \tau_1 - 1 \\ \tau_1 - 1 & -2 \end{pmatrix}, \quad \mathbf{H}_{1R} \equiv \frac{1}{2Pe} \begin{pmatrix} Pe(-1 + 2\lambda_0^1) & 1 - Pe\tau_2 \\ 1 - Pe\tau_2 & -2 \end{pmatrix}, \quad (73)$$

and

$$\mathbf{v}_{1L} \equiv \begin{pmatrix} v_1(0, t) \\ v_{1,x}(0, t) \end{pmatrix}, \quad \mathbf{v}_{1R} \equiv \begin{pmatrix} v_1(1, t) \\ v_{1,x}(1, t) \end{pmatrix}. \quad (74)$$

The eigenvalues of \mathbf{H}_{1L} are

$$\lambda\{\mathbf{H}_{1L}\} = \frac{1}{2}\lambda_0^1 + \frac{1}{4} - \frac{1}{2}\tau_1 - \frac{1}{2Pe} \pm \frac{1}{4Pe} \sqrt{\Delta_{1L}}, \quad (75)$$

where

$$\Delta_{1L} \equiv 4Pe^2(\lambda_0^1)^2 + 4Pe^2\lambda_0^1 - 8Pe^2\lambda_0^1\tau_1 + 8Pe\lambda_0^1 + Pe^2 - 4Pe^2\tau_1 + 4Pe + 4Pe^2\tau_1^2 - 8Pe\tau_1 + 8 - 8\tau_1 + 4\tau_1^2. \quad (76)$$

Some algebra reveals that these eigenvalues are non-positive if

$$2Pe + 1 - \sqrt{4Pe^2 + 2Pe - 4Pe\lambda_0^1} \leq \tau_1 \leq 2Pe + 1 + \sqrt{4Pe^2 + 2Pe - 4Pe\lambda_0^1}. \quad (77)$$

Similarly, the eigenvalues of \mathbf{H}_{1R} are

$$\lambda\{\mathbf{H}_{1R}\} = \frac{1}{2}\lambda_0^1 - \frac{1}{4} - \frac{1}{2Pe} \pm \frac{1}{4Pe} \sqrt{\Delta_{1R}}, \quad (78)$$

where

$$\Delta_{1R} \equiv Pe^2 - 4\lambda_0^1 Pe^2 - 4Pe + 4Pe^2(\lambda_0^1)^2 + 8Pe\lambda_0^1 + 8 - 8\tau_2 Pe + 4\tau_2^2 Pe^2. \quad (79)$$

It is straightforward to show that (78) is non-positive for

$$\frac{1 - \sqrt{2Pe - 4Pe\lambda_0^1}}{Pe} \leq \tau_2 \leq \frac{1 + \sqrt{2Pe - 4Pe\lambda_0^1}}{Pe}. \quad (80)$$

The equation for v_2 is the same as the equation for v_1 but with λ_0^1 replaced by λ_0^2 . The stability analysis, therefore, is the same as well. It follows that the bounds (64) and (65) on τ_1 and τ_2 , respectively, are sufficient conditions for ensuring asymptotic stability of the Galerkin projection of the tubular reactor equations with a penalty enforcement of the boundary conditions (61). \square

4.2. Implementation of the tubular reactor convection-diffusion-reaction reduced order model

A scalar POD basis is built for each of the unknowns, y and θ :

$$y(x, t) \approx y_M(x, t) = \sum_{m=1}^M a_m^y(t) \phi_m^y(x), \quad (81)$$

$$\theta(x, t) \approx \theta_M(x, t) = \sum_{m=1}^M a_m^\theta(t) \phi_m^\theta(x). \quad (82)$$

The POD modes ϕ_m^y are constructed from snapshots of the concentration y only; the POD modes ϕ_m^θ are constructed from snapshots of the temperature θ only. Note that one could, as an alternative, construct a vector basis $\boldsymbol{\phi} \in \mathbb{R}^2$ from snapshots of the vector $(y, \theta)^T \in \mathbb{R}^2$. Numerical experiments reveal that employing scalar bases for each of the variables (81) and (82) yields a slightly more accurate ROM for a fixed number of degrees of freedom for this problem.

The ROM is constructed by projecting the y equation in (63) onto ϕ_j^y and the θ equation in (63) onto ϕ_j^θ in the L^2 inner product, for $j = 1, \dots, M$. Projecting the concentration equation onto the j th POD mode, the following expression is obtained, after performing an integration by parts on the diffusion term and substituting the modal representation of the concentration,

$$\begin{aligned} \dot{a}_j^y = & - \sum_{k=1}^M a_k^y \left\{ \frac{1}{Pe_M} \left(\frac{\partial \phi_k^y}{\partial x}, \frac{\partial \phi_j^y}{\partial x} \right) \right. \\ & + \left(\frac{\partial \phi_k^y}{\partial x}, \phi_j^y \right) + \frac{1}{Pe_M} \left[\frac{\partial \phi_k^y}{\partial x} \Big|_{x=1} \phi_j^y(1) - \frac{\partial \phi_k^y}{\partial x} \Big|_{x=0} \phi_j^y(0) \right] \\ & - \tau_1 \left(\phi_k^y(0) - \frac{1}{Pe_M} \frac{\partial \phi_k^y}{\partial x} \Big|_{x=0} \right) \phi_j^y(0) - \tau_2 \frac{\partial \phi_k^y}{\partial x} \Big|_{x=1} \phi_j^y(1) \Big\} \\ & - D \left(\mathcal{N}(\mathbf{u}_M), \phi_j^y \right), \end{aligned} \quad (83)$$

where $\mathcal{N}(\mathbf{u}_M)$ is defined in (56). Similarly, for the temperature equation

$$\begin{aligned} \dot{a}_j^\theta = & - \sum_{k=1}^M a_k^\theta \left\{ \frac{1}{Pe_H} \left(\frac{\partial \phi_k^\theta}{\partial x}, \frac{\partial \phi_j^\theta}{\partial x} \right) + \left(\frac{\partial \phi_k^\theta}{\partial x}, \phi_j^\theta \right) + \beta \left(\phi_i^\theta, \phi_j^\theta \right) \right. \\ & + \frac{1}{Pe_H} \left[\frac{\partial \phi_k^\theta}{\partial x} \Big|_{x=1} \phi_j^\theta(1) - \frac{\partial \phi_k^\theta}{\partial x} \Big|_{x=0} \phi_j^\theta(0) \right] \\ & - \tau_1 \left(\phi_k^\theta(0) - \frac{1}{Pe_H} \frac{\partial \phi_k^\theta}{\partial x} \Big|_{x=0} \right) \phi_j^\theta(0) - \tau_2 \frac{\partial \phi_k^\theta}{\partial x} \Big|_{x=1} \phi_j^\theta(1) \Big\} \\ & + \beta(1 - \theta_0, \phi_j^\theta) + BD \left(\mathcal{N}(\mathbf{u}_M), \phi_j^\theta \right). \end{aligned} \quad (84)$$

In total, there are $2M$ unknowns $\{a_j^y, a_j^\theta : j = 1, \dots, M\}$. To estimate a desirable range of τ_1 and τ_2 , a stable point (y_0, θ_0) in the vicinity of the limit cycle is selected, and the result of Theorem 4.1.1 is applied (Section 4.3).

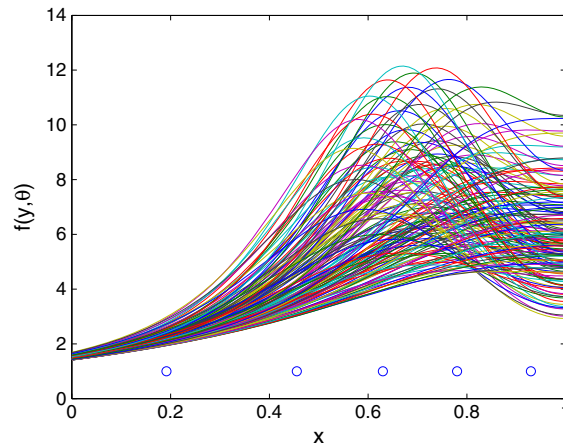


Figure 8. $\mathcal{N}(\mathbf{u})$ (56) (solid lines) and interpolation points (circles) for the tubular reactor convection-diffusion-reaction system (proper orthogonal decomposition basis, $M = 5$).

Both systems (83) and (84) contain the following non-linearity:

$$(\mathcal{N}(\mathbf{u}_M), \phi_j) = \left(\left(\sum_{m=1}^M a_m^y(t) \phi_m^y(x) + 1 \right) \exp \left\{ \frac{\gamma \sum_{m=1}^M a_m^\theta(t) \phi_m^\theta(x)}{\sum_{m=1}^M a_m^\theta(t) \phi_m^\theta(x) + 1} \right\}, \phi_j \right), \quad (85)$$

which clearly cannot be pre-computed prior to time integration of the ROM and hence must be recomputed at each time step of the time-integration scheme employed with the ‘direct’ treatment of the non-linearity (85). This approach is extremely costly. However, the interpolation outlined in Section 2.2 can be employed to recover efficiency of the ROM^{††}. The interpolation points computed for the scalar function $\mathcal{N}(\mathbf{u})$ (56) with $M = 5$ are plotted in Figure 8 along with this non-linear function shown for different times t .

4.3. Numerical results for the tubular reactor convection-diffusion-reaction system

The high-fidelity solution to the tubular reactor CDR system was obtained using a Fourier spectral Galerkin method in space and a fourth order Runge–Kutta time-integration scheme. The domain

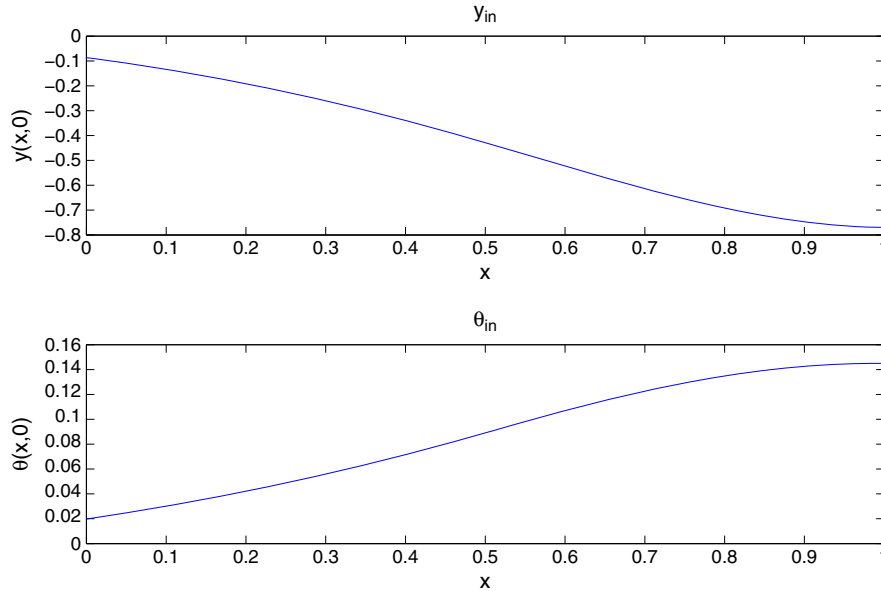


Figure 9. Initial concentration and temperature profiles y_{in} and θ_{in} for the tubular reactor convection-diffusion-reaction system.

Table I. Fluid properties used in the high-fidelity numerical solution of (49)–(52) from which snapshots were taken.

| Property | Symbol | Value |
|---|------------|-------|
| Péclet number for heat transfer | Pe_H | 5.00 |
| Péclet number for mass transfer | Pe_M | 5.00 |
| Dimensionless heat of reaction | B | 0.50 |
| Dimensionless activation energy | γ | 25.0 |
| Dimensionless heat transfer coefficient | β | 2.50 |
| Damköhler number | D | 0.17 |
| — | θ_0 | 1 |

^{††}Note that the current model is a variant of the CDR tubular reactor model developed in [10] but is more efficient, as the BPIM is employed to handle the highly non-linear term appearing in the equation. In [10], the terms involving the projection (85) are treated directly.

$\Omega = (0, 1)$ was discretized by $N = 101$ spatial discretization points so that $\Delta x = 0.01$. The initial conditions y_{in} and θ_{in} , plotted in Figure 9, were calculated using an implicit relation scheme for the steady state solution. The values of the parameters for the solution from which the snapshots were taken are summarized in Table I. For a value of the Damkhöler number in the range $0.165 \leq D \leq 0.17$, the solution is known to exhibit a stable limit cycle (Figure 13). A total of 100 snapshots were taken from this simulation for which $D = 0.17$. These snapshots were saved every $\Delta t_{\text{snap}} = 0.25$ up to time $T = 25$. From these snapshots, the POD modes to be used in the ROM were computed. The first four POD modes for the concentration and temperature are plotted in Figure 10.

In the first test performed, a POD ROM with five concentration and five temperature modes (so that $2M = 10$) and with $D = 0.17$ is evaluated. The ROM is run until time $T = 100$. Note that this is a much longer time horizon than the time horizon used in the high-fidelity simulation from which the POD basis was generated and well into the stable limit cycle regime (Figure 11). The objective here is to test the predictive capability of the ROM for long time simulations. Figure 11 shows the limit cycles in the concentration and temperature (the solutions $y(1, t)$ and $\theta(1, t)$ as a function of time) compared with the limit cycles produced by the high-fidelity simulation for two ROMs: an ROM built using a ten mode (five concentration and five temperature modes) POD basis with a direct treatment of the non-linear terms (plotted in blue), and an ROM built using a ten mode (five concentration and five temperature modes) POD basis with interpolation of the non-linear terms (plotted in red). The boundary conditions in both ROMs are imposed via the penalty formulation outlined in Section 4.1 with $\tau_1 = \tau_2 = 105$. These values are within the stability range derived in Theorem 4.1.1 for a linearization point (y_0, θ_0) with $y_0 \approx -1$ and $\theta_0 > 0.45$, which is in the vicinity of the stable limit cycle. Both ROMs capture the oscillatory behavior exhibited by the solution (the limit cycle). The red and blue curves in Figure 11 are indistinguishable, which suggest that the amount of error introduced into the approximation from the interpolation of the non-linear terms is not significant. This observation is confirmed by Figure 12, which shows the pointwise, time-average errors (48) in the concentration y and temperature θ relative to the high-fidelity solution as a function of space with $\tau_1 = \tau_2 = 105$ and $2M = 10$ (five concentration and five temperature) modes. The error is maximal near the right boundary $x = 1$, where a Neumann boundary condition is imposed. Figure 11 shows that the limit cycle behavior of the solution is nonetheless captured quite well by

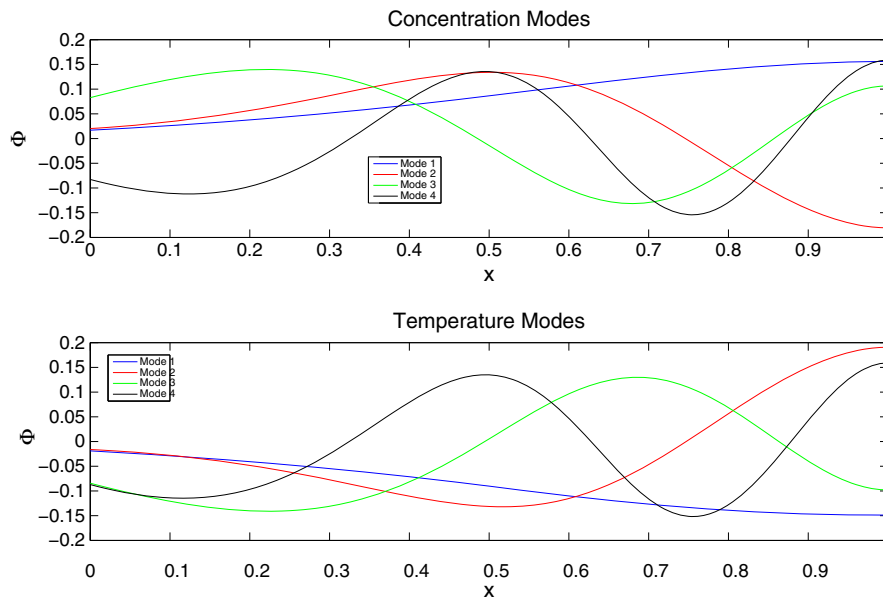


Figure 10. Concentration and temperature proper orthogonal decomposition modes for the tubular reactor convection-diffusion-reaction system.

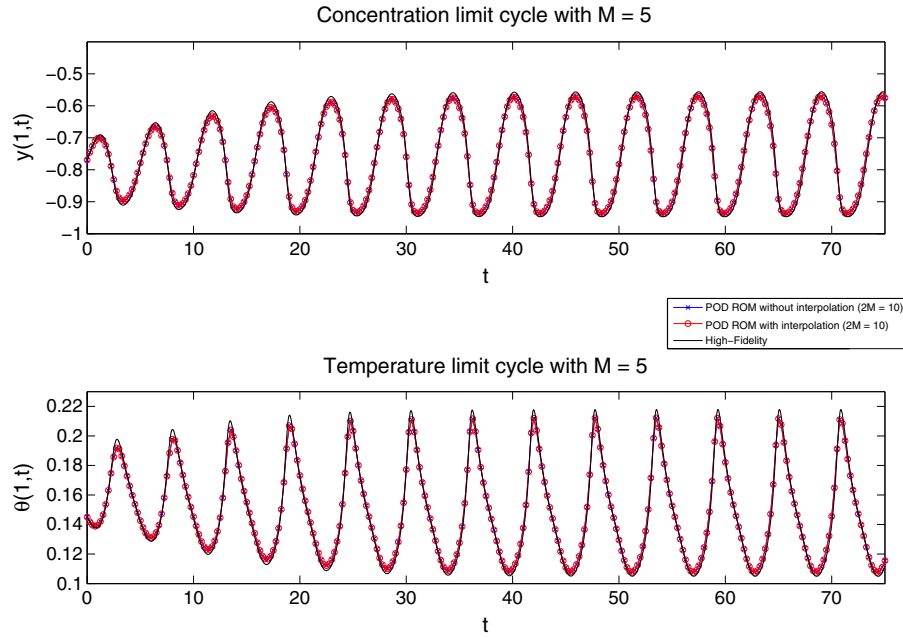


Figure 11. Illustration of limit cycles (y and θ at $x = 1$ as a function of time t) for different reduced order models (ROM) for the tubular reactor convection-diffusion-reaction system with $2M = 10$ (five concentration and five temperature) modes, $\tau_1 = \tau_2 = 105$ (without and with interpolation). POD, proper orthogonal decomposition.

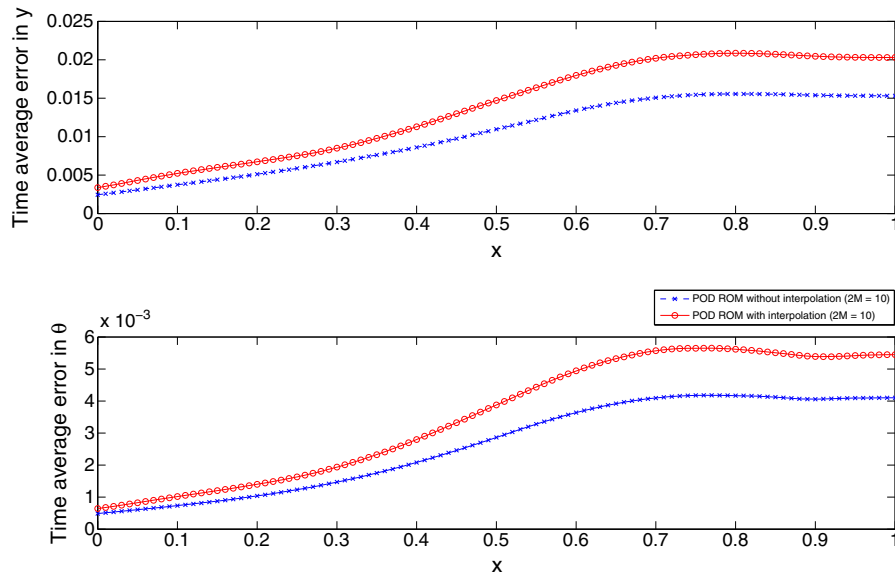


Figure 12. Time-average errors (48) in the reduced order model solutions solution for the tubular reactor convection-diffusion-reaction system with $2M = 10$ (five concentration and five temperature) proper orthogonal decomposition modes, $\tau_1 = \tau_2 = 105$.

the ROMs even at this point of maximal error. The ROM solution with interpolation is slightly less accurate than the ROM solution computed via the direct approach but only by a very small margin. In the second test performed, the predictive capability of the ROM with respect to changes in the Damkhöler number is assessed. It is of particular interest whether the ROM can reproduce the bifurcation diagram for this problem. Using the same ten (five concentration and five temperature) mode POD basis described previously, computed from snapshots taken up to time $T = 25$ and with

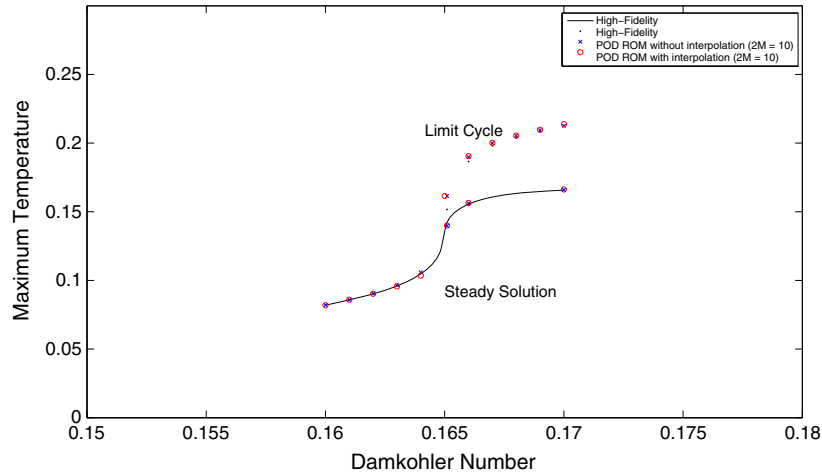


Figure 13. Bifurcation diagram showing the existence of stable oscillatory solutions to the tubular reactor convection-diffusion-reaction system when $Pe_H = Pe_M = 5$, $B = 0.5$, $\gamma = 25$, $\beta = 2.5$, $\theta_0 = 1$.

$D = 0.17$, solutions to (49) with the boundary conditions (50) and (51) are computed using the ROM for different values of D . Again, the ROMs are run for a longer time until $T = 100$. Figure 13 compares the bifurcation diagrams obtained for this problem using the high-fidelity model, the ROM without interpolation, and the ROM with interpolation. The reader can observe that both ROMs predict correctly the existence of stable oscillatory solutions as a function of the Damköhler number and identify the lower Hopf bifurcation point $D = 0.165$. The error in the maximum temperature computed by the ROM relative to the maximum temperature computed by the high-fidelity model is, in general, less than 5% for each value of D . It is interesting to observe that a ROM computed from the snapshots taken in an oscillatory regime can still capture well non-oscillatory solutions in the steady regime. Plots of the ROM solutions for $D \neq 0.17$ are not shown here for the sake of brevity.

5. CONCLUSIONS

A technique for building efficient POD/Galerkin ROMs for non-linear IBVPs whose solutions exhibit inherently non-linear behaviors such as metastability and periodic regimes (limit cycles) has been developed. Because the ROM is built by projecting the continuous governing equations onto a set of basis modes rather than their discretized analogs, enforcement of the boundary conditions by the ROM solution is not automatic. It is observed that the POD modes do not, in general, satisfy the boundary conditions, particularly if the boundary conditions are of the inhomogeneous, mixed and/or Robin kind. A formulation in which the boundary conditions are enforced weakly via the penalty method is derived. To determine appropriate values of the penalty parameters, an asymptotic stability analysis of the Galerkin scheme with penalty-enforced boundary conditions is performed, following a linearization and localization of the equations about a stable steady state similar to the technique employed in [19]. This analysis, borrowed from the spectral method community and performed at the level of the governing (continuous) equations, is made possible by the fact that the *continuous* projection approach is employed in building the ROM. It is emphasized that the same *a priori* stability may not be guaranteed, in general, for a ROM constructed using the discrete projection approach [25, 26]. As stability is an essential mathematical property of any discretization, including a ROM, and the continuous projection approach can guarantee these results *a priori*, ROMs based on this proposed approach are recommended by the authors despite the additional programming required in implementing such a ROM. Asymptotically stable ROMs with stability-preserving penalty boundary treatment are developed for the Allen–Cahn (or ‘bistable’) equation as well as a CDR system representing a tubular reactor. Efficiency of these non-linear ROMs is maintained by using the BPIM to handle the projection of the non-linear terms that are

present in these equations. The ROMs, both without as well as with interpolation, are stable and capture the correct non-linear dynamics of the solutions, namely the phenomenon of metastability for the Allen–Cahn equation and a stable limit cycle for the CDR system.

It is emphasized that the model reduction approach and stability analysis technique proposed herein and illustrated specifically on the two model problems considered can be used to build stable, efficient, and accurate ROMs for other non-linear equations in a plethora of applications, following the approach outlined in Section 2.4. The reader is referred to [14] for a discussion of the application of the approach to the compressible Navier–Stokes equations (and other conservation laws) and to [12] for a discussion of a stability-preserving discrete implementation of a ROM constructed using the continuous projection approach in two and three spatial dimensions.

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